

### Exact preservation of the free energy in a modified Migdal-Kadanoff approximation

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The simple, but *ad hoc*, prescription for bond shifting in the Migdal-Kadanoff approximation is replaced by a systematic calculational procedure. In this method, the free energy is required to be preserved exactly by means of matching series expansions. The resulting renormalization group is characterized by a small parameter, and can be extended by working to higher order. A significant quantitative improvement over the standard Migdal-Kadanoff method is obtained with little increase in calculational effort. This approach is ultimately limited, however, by being restricted to a one-dimensional interaction parameter space.

The fundamental problem of statistical mechanics is to evaluate the free energy, but since it is generally not possible to do this exactly, approximate methods must be used. In the Migdal-Kadanoff<sup>1</sup> (MK) approximate renormalization-group technique, the free energy of the calculation is known rigorously to be a lower bound to the exact free energy of the system. The MK approximation is easy to implement and thus has enjoyed wide usage; however, the quantitative level of accuracy is rather low. To improve the calculation, several modifications have been studied,<sup>2</sup> often involving a free parameter which is adjusted to optimize the bound on the free energy.<sup>3</sup> In this paper, we study a new implementation of the basic MK scheme in which the free energy is actually preserved exactly through a given order in a high- or low-temperature series expansion. Thus, we are able to develop a position-space renormalization-group transformation which is characterized by a small parameter, in contrast to the usual situation, and is still very simple to utilize. Quantitative results are markedly improved over the MK method, though, as is shown below, the restriction of the calculation to a one-dimensional parameter space will ultimately limit this approach. In what follows we first briefly recapitulate the basic MK approximation, then explore the consequences of preserving the free energy exactly.

For clarity, we study the simple nearest-neighbor Ising model, though this same approach can be extended to more complex systems as well. Thus, consider the reduced Hamiltonian,

$$-\beta\mathcal{H}(K; \{s\}) = K \sum_{\langle ij \rangle} s_i s_j, \tag{1}$$

where  $s_i = \pm 1$ , and  $K > 0$  corresponding to a ferromagnetic interaction. Figure 1(a) displays the ori-

ginal system on a two-dimensional ( $d=2$ ) square lattice, characterized by  $N$  spins and a reduced free energy

$$f(K) = \frac{1}{N} \ln \sum_{\{s\}} e^{-\beta\mathcal{H}(K; \{s\})}. \tag{2}$$

The goal is to calculate this free energy, and in the MK approach this is carried out in two steps. The first is to restructure the original lattice by moving away some of the bonds, and strengthening those bonds that remain, so that the lattice of Fig. 1(b) is obtained. This lattice again has  $N$  spins, but the free energy now has a different functional form, which we denote by  $\tilde{f}(\tilde{K})$ , where  $\tilde{K}$  represents the strengthened couplings. The prescription followed by MK is to require that the total bond strength of the restructured lattice be equal to that of the origi-

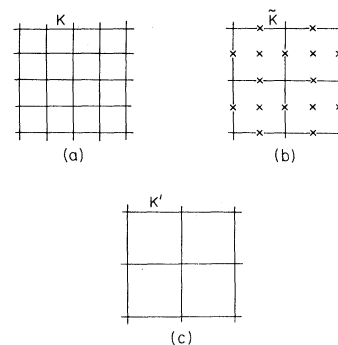


FIG. 1. (a) Lattice of original system with nearest-neighbor coupling  $K$ . (b) Restructured lattice with strengthened couplings  $\tilde{K}$ . (c) Result of decimating out the variables labeled by crosses in (b). This lattice is identical to the original, but with lengths rescaled by a factor of 2 ( $b=2$ ) and couplings renormalized to  $K'$ . In MK,  $\tilde{K} = b^{d-1}K$ ; in this approach  $\tilde{K}$  is a function of  $K$  determined so as to preserve the free energy.

nal lattice. For example, in this case it is clear that the number of bonds in Fig. 1(b) is half the number of bonds in Fig. 1(a), and thus  $\tilde{K}$  is taken to be twice the strength of  $K$ . In general, if all lengths are rescaled by a factor of  $b$  on a  $d$ -dimensional hypercubic lattice, then  $\tilde{K}/K = b^{d-1}$  ( $b=2$  in this example). Of course, this procedure of requiring the total bond strength to be preserved is entirely *ad hoc* and introduces an error whose magnitude is uncontrolled. It is important to note that the approximate nature of the MK method is due solely to this restructuring step.

The second step of the calculation is to trace over those degrees of freedom labeled by crosses in Fig. 1(b). This decimation transformation can be carried out exactly, and results in the system shown in Fig. 1(c)—note that the lattice constant is now twice that of the original, and thus  $b=2$ . This lattice has  $N' = b^{-d}N$  spins and a free energy  $f(K')$ , that is, the same functional form as in the original system, but with a renormalized coupling  $K'$ . The expression for  $K'$  is easily derived and can be written as

$$K'(K) = \frac{1}{2} \ln \left[ \frac{\lambda_+^b + \lambda_-^b}{\lambda_+^b - \lambda_-^b} \right], \quad (3)$$

where

$$\lambda_{\pm} = e^{\tilde{K}_{\pm}} e^{-\tilde{K}}, \quad (4)$$

and  $\tilde{K} = b^{d-1}K$ . In addition, the decimation generates a contribution to the free energy given by

$$K'_0(K) = \frac{1}{2} \ln \left[ \frac{\lambda_+^{2b} - \lambda_-^{2b}}{4} \right]. \quad (5)$$

This completely defines the MK renormalization-group transformation.

Returning now to the first step of the transformation, the lattice restructuring, we seek to go beyond the *ad hoc* prescription of MK by introducing a more systematic approach. Instead of simply requiring the total bond strength to be the same in the original and restructured lattices, we specify that the free energy be preserved to a given order in a series expansion. For example, if the free energy is given by  $f(K) = \sum_n a_n K^n$ , the MK relationship  $\tilde{K}/K = b^{d-1}$  is replaced by  $\tilde{K}(K)/K = \sum_n b_n K^n$  where the  $b_n$  are chosen so that the calculated free energy matches the coefficients  $a_n$ . The function  $\tilde{K}(K)$  then defines the recursion relations through Eqs. (3) and (4), and the rest of the calculation proceeds as before. Notice that  $\tilde{K}(K)$  can be totally analytic and still the renormalization-group machinery produces singular behavior. Thus, by approximating a fairly simple function like  $\tilde{K}(K)$ ,

and then using the renormalization-group apparatus to generate singularities, such an approach can produce improved approximate recursion relations. In practice, one finds that only the first few terms in an expansion of  $f(K)$  need be kept in order to achieve a substantial improvement over MK. The resulting approximation is characterized by the expansion parameter of the free energy, and can be systematically improved by working to higher order. Thus, the uncontrolled nature of the original MK method is replaced by a definite calculational scheme, the results of which are now examined.

To illustrate the approach in practice, we carry out the program for various limits. First, when  $K \rightarrow \infty$  we have the result

$$\lim_{K \rightarrow \infty} f(K) = \frac{1}{2} qK, \quad (6)$$

where  $q$  is the coordination number of the lattice. The free energy for the restructured lattice,  $\tilde{f}(\tilde{K})$ , takes on a similar form, namely,

$$\lim_{\tilde{K} \rightarrow \infty} \tilde{f}(\tilde{K}) = \frac{1}{2} qb^{-(d-1)}\tilde{K} + a \ln 2, \quad (7)$$

where

$$a = 1 - b^{-d} [1 + \frac{1}{2}q(b-1)]. \quad (8)$$

The term  $a \ln 2$  takes into account the disconnected spins in Fig. 1(b). Now, by setting  $\tilde{f}(\tilde{K})$  equal to  $f(K)$  through this order, we obtain

$$\lim_{K \rightarrow \infty} \frac{\tilde{K}(K)}{K} = b^{d-1} \left[ 1 - \frac{2a \ln 2}{qK} \right]. \quad (9)$$

Note that the MK prescription of  $\tilde{K}/K = b^{d-1}$  is recovered in this limit, though the approach to this result varies from one system to another depending on the value of  $a$ . For example, on a triangular lattice with  $b=2$  no disconnected spins result from the restructuring transformation,<sup>4</sup> and thus  $a=0$ . Therefore, even to lowest order this method distinguishes between the square and triangular lattices, whereas the MK transformation does not.

While the MK prescription is approached in the limit  $K \rightarrow \infty$ , the results are quite different for  $K \rightarrow 0$ . In this case, the free energy expansion is

$$\begin{aligned} \lim_{K \rightarrow 0} f(K) &= \ln 2 + d \ln(\cosh K) \\ &+ \frac{d(d-1)}{2} v^4 + \dots \\ &= \ln 2 + d \left( \frac{1}{2} K^2 - \frac{1}{12} K^4 \right) \\ &+ \frac{d(d-1)}{2} K^4 + O(K^6), \end{aligned} \quad (10)$$

where  $v = \tanh K$ , and similarly,

$$\begin{aligned} \lim_{\tilde{K} \rightarrow 0} \tilde{f}(\tilde{K}) &= \ln 2 + db^{-(d-1)} \ln(\cosh \tilde{K}) \\ &+ b^{-d} \frac{d(d-1)}{2} \tilde{v}^8 + \dots \\ &= \ln 2 + db^{-(d-1)} \left( \frac{1}{2} \tilde{K}^2 - \frac{1}{12} \tilde{K}^4 \right) \\ &+ O(\tilde{K}^6), \end{aligned} \tag{11}$$

with  $\tilde{v} = \tanh \tilde{K}$ . From these expressions, preservation of the free energy requires that

$$\lim_{K \rightarrow 0} \frac{\tilde{K}(K)}{K} = b^{(d-1)/2} (1 + \alpha K^2) + O(K^4), \tag{12}$$

where

$$\alpha = \frac{6(d-1) + b^{(d-1)} - 1}{12}.$$

So, in this limit,  $\tilde{K}/K$  simply approaches the square root of the usual MK result; the full form must therefore interpolate between these two limits as  $K$  is varied (see Fig. 3). The fact that  $\tilde{K}/K = b^{(d-1)/2}$  is required as  $K \rightarrow 0$  rather than  $b^{d-1}$  means that the free energy calculated in the MK approximation will actually start off with the wrong curvature. Finally, note that the expansion for  $\tilde{K}(K)/K$  is even in  $K$ , reflecting the fact that for the square lattice the free energy itself is even, i.e.,  $f(K) = f(-K)$ . For the triangular lattice this is no longer true, and then one finds that all positive powers of  $K$  are included in  $\tilde{K}(K)/K$ , again distinguishing the two lattices.

To this point, we have expanded the free energy only to very low order, but, of course, it is straightforward to extend the calculation by including more terms and thus determine a more accurate expression for  $\tilde{K}(K)/K$ . The error produced in the free energy from such a calculation is shown in Fig. 2, where it is compared with the corresponding error from the MK method. The upper half of the figure presents the MK results, with a maximum error, at the critical point  $K_c \approx 0.4407$ , of approximately 20%. In the bottom half of the figure errors from the present calculation are shown; note, however, that the scale is reduced by a factor of 10 from that used for MK. Thus, for example, by preserving the free energy to order  $v^4$  from high temperature—and correspondingly to order  $(e^{-2K})^4$  from low temperature—the maximum error is only about  $-2\%$ , whereas by working to order  $v^8$  the largest error is reduced to  $-0.5\%$ . As more orders are included in  $\tilde{K}(K)/K$ , the calculation rapidly becomes extremely accurate. Also, note that as  $K$  is in-

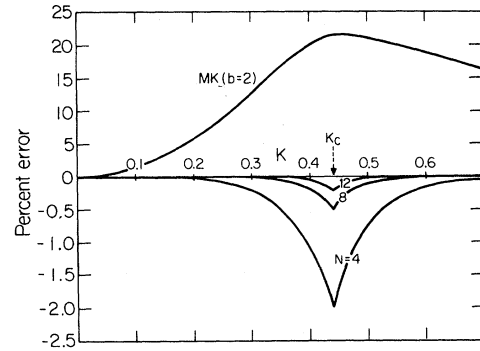


FIG. 2. Percentage error in the approximate free energy as a function of  $K$  for  $b=2$ . Upper half of the figure displays the MK result. Lower half shows the present calculation—but with a scale reduced by a factor of 10.  $N$  denotes the order to which the free energy has been preserved, and  $K_c$  locates the Ising critical point.

creased from zero, the MK error starts up immediately, while the series-expansion results have no appreciable error until  $K$  is increased considerably. This reflects the fact that the MK free energy has an incorrect initial curvature, as mentioned above.

The function  $\tilde{K}(K)/K$  that results from preserving the free energy to order  $v^{40}$  (Ref. 5) is plotted as a function of  $K$  in Fig. 3, and, to within the accuracy of the plot, this can be considered as the exact result. The corresponding approximate free energy has an error which is never more than  $-0.02\%$ . Notice in Fig. 3 the amount of deviation from MK

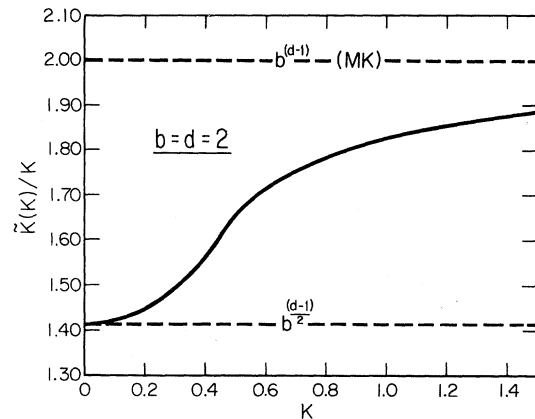


FIG. 3.  $\tilde{K}(K)/K$  as a function of  $K$  for the Ising model on a square lattice.  $\tilde{K}(K)$  is determined so that the exact and approximate free energies match to order  $(\tanh K)^{40}$  and  $(e^{-2K})^{40}$ . This result is indistinguishable from what would be obtained by preserving the free energy exactly to all orders. Dashed lines represent the asymptotic limits for  $b=2$  and  $K \rightarrow 0, \infty$ . Note that the MK prescription always overstrengthens the bonds.

required for the free energy to be preserved, and that this will be greater the larger  $b$  and  $d$ . Note also that the MK prescription always overcompensates for the bond shifting by making the remaining bonds too strong.

Clearly, even to very low order this approach produces a marked improvement in the approximate free energy. The fixed-point properties are also considerably better than in ordinary MK. In particular, the results obtained by using  $\tilde{K}(K)/K$  as shown in Fig. 3 are  $K^*=0.5006$  [as compared to 0.4407 (exact<sup>6</sup>) and 0.305 (MK)] and  $\nu=1.11$  [1.0 (exact<sup>6</sup>) and 1.34 (MK)]. These results are obtained with a rescaling factor of  $b=2$ , but by going to the infinitesimal rescaling limit, that is  $b \rightarrow 1$ , further improvement develops. We again require the free energy to be preserved, in which case the condition for a fixed point can be written

$$f(K^*) = \left. \frac{\partial K'_0(K^*)}{\partial b} \right|_{b=1} = \frac{1}{4}(\lambda_+^2 \ln \lambda_+ - \lambda_-^2 \ln \lambda_-). \quad (13)$$

In Fig. 4(a) the results for the fixed point  $K^*$  are shown as a function of  $1/N$ , where  $N$  is the highest order of  $\nu$  (and  $e^{-2K}$ ) that is preserved in the free energy. It is clear that convergence is rapid, just as it is for the free energy in Fig. 2. For the exponent  $\nu$  we have

$$\nu = \left. \frac{1}{\frac{\partial}{\partial b} \left[ \frac{\partial K'}{\partial K} \right]_{K^*}} \right|_{b=1}, \quad (14)$$

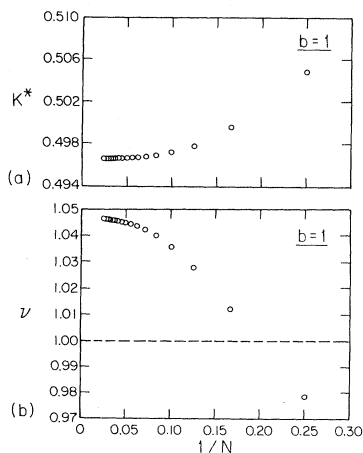


FIG. 4. Results for infinitesimal rescaling,  $b \rightarrow 1$ . (a)  $K^*$  as a function of  $1/N$ , where  $N$  is the order to which the free energy is preserved. Notice the rapid convergence, though the exact value of  $K_c=0.4407$  is not obtained. (b) Critical exponent  $\nu$  vs  $1/N$ . Dashed line indicates the exact result.

and the corresponding results are displayed in Fig. 4(b). Thus, extending the calculation to higher order results in a rapid and systematic convergence to the values,  $K^*=0.4965$  and  $\nu=1.046$ . These results are a definite improvement over the standard MK calculation, but still we see that even if the free energy is preserved exactly, the limiting fixed-point properties will not recover the exact values.

We can demonstrate this by considering the consequences of preserving the free energy exactly through all orders. So far, we have concentrated only on the restructuring step of the transformation, and thus on the relation of  $\tilde{K}$  to  $K$ ; but if we now perform the exact decimation of the second step we can express the function  $\tilde{f}(\tilde{K})$  in terms of the original free energy  $f$ . The result is

$$\tilde{f}(\tilde{K}) = a \ln 2 + \frac{1}{2} q b^{-d} K'_0 + b^{-d} f(K'), \quad (15)$$

where  $a$ ,  $K'$ , and  $K'_0$  are as defined above. For simplicity consider the case  $b=d=2$ , as in Fig. 1, for which  $K'_0 = \ln 2 + K'$  and the condition  $\tilde{f}(\tilde{K}) = f(K)$  becomes

$$f(K) = \frac{3}{4} \ln 2 + \frac{1}{2} K' + \frac{1}{4} f(K'), \quad (16)$$

implicitly defining the relation  $K'(K)$ . From this we can see that the fixed point is given by

$$K^* = \frac{3}{2} [f(K^*) - \ln 2]. \quad (17)$$

It is apparent that  $K^* \neq K_c$ , since  $K_c$  and  $f(K_c)$  do not obey such a simple relationship. In fact, using exact results for the two-dimensional Ising-model free energy we find  $K^*$  is as given above for  $b=2$ , namely  $K^*=0.5006$ . Similarly, we can linearize about the fixed point to obtain

$$\left. \frac{\partial K'}{\partial K} \right|_{K^*} = \frac{2 \left. \frac{\partial f}{\partial K} \right|_{K^*}}{1 + \left. \frac{\partial f}{\partial K} \right|_{K^*}}. \quad (18)$$

Again, using exact results for  $\partial f/\partial K$  we find  $\nu=1.11$ . The cause of these discrepancies can readily be seen by considering Eq. (16) as  $K \rightarrow K_c$ . In this case the left-hand side of the equation,  $f(K)$ , becomes singular—but there is no corresponding singularity on the right-hand side of the equation since  $K'(K_c) \neq K_c$ . The only way for the right-hand side of Eq. (16) to be singular at  $K_c$  is for  $K'(K)$  itself to be singular there. Thus, preserving the free energy exactly, while restricting the calculation to a one-dimensional parameter space, results in a recursion relation which is nonanalytic and whose critical properties need not agree with the exact values.

Fortunately, the singularities in  $K'(K)$  and  $\tilde{K}(K)$  are weak and thus the final results are still rather good.

Therefore, even though the utility of this approach is ultimately diminished somewhat by working with only a single interaction parameter, the approximate results represent an improvement over the basic MK method. These results also suggest other simple extensions of MK. For example, we have seen that the MK procedure always overstrengthens the bonds, so one way to improve the calculation is simply to reduce this strengthening factor. In the simplest case, we can require that  $\tilde{K}/K$  be a constant, and then adjust this constant between the limits  $b^{d-1}$  and  $b^{(d-1)/2}$  until some known exact result is recovered. This is a simple modification, but can result in good quantitative results,<sup>7</sup> even for  $d=3$ . At the expense of introducing more parameters in  $\tilde{K}(K)/K$  one can easily write an analytic interpolating form that attains the correct limits for high and low temperature, and excellent results for intermediate temperatures.

To recapitulate, the present method is based on preserving the free energy of the system exactly through some order in a series expansion. As a result, the bond strength of the restructured lattice,  $\tilde{K}$ ,

becomes a function of  $K$  which interpolates between the MK result for  $K \rightarrow \infty$  and the square root of this value for  $K \rightarrow 0$ . If the free energy is preserved exactly to all orders in this scheme,  $\tilde{K}(K)$  develops singularities which are due to forcing the system to remain in the limited parameter space of homogeneous nearest-neighbor couplings only. If an enlarged parameter space is utilized, as in the Kadanoff variational method for instance, then such a scheme of preserving the free energy has a better chance of succeeding. An interesting example is the exact differential renormalization group of Hilhorst, Schick, and van Leeuwen,<sup>8</sup> where the interactions, which are only nearest neighbor, nonetheless depend continuously on position so that each bond takes on a different value. In this sense the parameter space is infinite, and preserving the exact free energy produces analytic recursion relations with the correct critical properties.

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<sup>1</sup>A. A. Migdal, Zh. Eksp. Teor. Fiz. **69**, 810 (1975) [Sov. Phys.—JETP **42**, 413, (1975)]; **69**, 1457 (1975) [**42**, 743 (1975)]; L. P. Kadanoff, Ann. Phys. (NY), **100**, 359 (1976).

<sup>2</sup>R. Lipowsky, J. Phys. A **15**, L19 (1982); S. Caracciolo, Nucl. Phys. B **180**, 405 (1981); S. Caracciolo, G. Parisi, and N. Sourlas (unpublished).

<sup>3</sup>R. H. Swendsen and R. K. P. Zia, Phys. Lett. **69A**, 382 (1979).

<sup>4</sup>A. N. Berker, S. Ostlund, and F. A. Putnam, Phys. Rev. B **17**, 3650 (1978).

<sup>5</sup>C. Domb, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and M. S. Green (Academic, New York, 1974), Vol. 3.

<sup>6</sup>L. Onsager, Phys. Rev. **65**, 17 (1944).

<sup>7</sup>J. S. Walker and C. A. Vause, Phys. Lett. **79A**, 421 (1980), and in *the Proceedings of the Eighth Symposium on Thermophysical Properties, 1981*, edited by J. V. Sengers (American Society of Mechanical Engineers, New York, 1982), Vol. 1, pp. 411–418.

<sup>8</sup>H. J. Hilhorst, M. Schick, and J. M. J. van Leeuwen, Phys. Rev. Lett. **40**, 1605 (1978); Phys. Rev. B **19**, 2749 (1979).